Alfonso Pedone

List of Publications by Citations

130 papers	4,167 citations	38 h-index	58 g-index
135 ext. papers	4,710 ext. citations	4 avg, IF	5.83 L-index

#	Paper	IF	Citations
130	A new self-consistent empirical interatomic potential model for oxides, silicates, and silica-based glasses. *Journal of Physical Chemistry B*, **2006**, 110, 11780-95	3.4	362
129	Role of Solvent on Charge Transfer in 7-Aminocoumarin Dyes: New Hints from TD-CAM-B3LYP and State Specific PCM Calculations. *Journal of Chemical Theory and Computation*, **2013**, 9, 4087-96	6.4	115
128	New Insights into the Atomic Structure of 45S5 Bioglass by Means of Solid-State NMR Spectroscopy and Accurate First-Principles Simulations. *Chemistry of Materials*, **2010**, 22, 5644-5652	9.6	112
127	Properties Calculations of Silica-Based Glasses by Atomistic Simulations Techniques: A Review. *Journal of Physical Chemistry C*, **2009**, 113, 20773-20784	3.8	104
126	Insight into Elastic Properties of Binary Alkali Silicate Glasses; Prediction and Interpretation through Atomistic Simulation Techniques. *Chemistry of Materials*, **2007**, 19, 3144-3154	9.6	102
125	Molecular Dynamics Studies of Stress−Strain Behavior of Silica Glass under a Tensile Load. *Chemistry of Materials*, **2008**, 20, 4356-4366	9.6	93
124	Elucidation of the structural role of fluorine in potentially bioactive glasses by experimental and computational investigation. *Journal of Physical Chemistry B*, **2008**, 112, 12730-9	3.4	92
123	Evidence of catalase mimetic activity in Ce(3+)/Ce(4+) doped bioactive glasses. *Journal of Physical Chemistry B*, **2015**, 119, 4009-19	3.4	89
122	Computational Insight into the Effect of CaO/MgO Substitution on the Structural Properties of Phospho-Silicate Bioactive Glasses. *Journal of Physical Chemistry C*, **2009**, 113, 15723-15730	3.8	82
121	The structure of fluoride-containing bioactive glasses: new insights from first-principles calculations and solid state NMR spectroscopy. *Journal of Materials Chemistry*, **2012**, 22, 12599		78
120	Role of Magnesium in Soda-Lime Glasses: Insight into Structural, Transport, and Mechanical Properties through Computer Simulations. *Journal of Physical Chemistry C*, **2008**, 112, 11034-11041	3.8	73
119	Fluorine environment in bioactive glasses: ab initio molecular dynamics simulations. *Journal of Physical Chemistry B*, **2011**, 115, 2038-45	3.4	70
118	Quantitative structure-property relationships of potentially bioactive fluoro phospho-silicate glasses. *Journal of Physical Chemistry B*, **2009**, 113, 10331-8	3.4	67
117	Computational simulations of solid state NMR spectra: a new era in structure determination of oxide glasses. *RSC Advances*, **2013**, 3, 10550	3.7	66
116	FFSiOH: a New Force Field for Silica Polymorphs and Their Hydroxylated Surfaces Based on Periodic B3LYP Calculations. *Chemistry of Materials*, **2008**, 20, 2522-2531	9.6	65
115	Absorption and emission UV-Vis spectra of the TRITC fluorophore molecule in solution: a quantum mechanical study. *Physical Chemistry Chemical Physics*, **2010**, 12, 1000-6	3.6	64
114	Multinuclear NMR of CaSiO(3) glass: simulation from first-principles. *Physical Chemistry Chemical Physics*, **2010**, 12, 6054-66	3.6	64

113	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	63
112	Competitive Binding of Proteins to Gold Nanoparticles Disclosed by Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2015**, 119, 22172-22180	3.8	61
111	Extension of the AMBER force-field for the study of large nitroxides in condensed phases: an ab initio parameterization. *Physical Chemistry Chemical Physics*, **2010**, 12, 11697-709	3.6	58
110	Void size distribution in MD-modelled silica glass structures. *Journal of Non-Crystalline Solids*, **2006**, 352, 285-296	3.9	58
109	Benchmarking TD-DFT against Vibrationally Resolved Absorption Spectra at Room Temperature: 7-Aminocoumarins as Test Cases. *Journal of Chemical Theory and Computation*, **2015**, 11, 5371-84	6.4	57
108	Realistic Modeling of Fluorescent Dye-Doped Silica Nanoparticles: A Step Toward the Understanding of their Enhanced Photophysical Properties.. *Chemistry of Materials*, **2011**, 23, 5016-5023	9.6	56
107	Probing silicon and aluminium chemical environments in silicate and aluminosilicate glasses by solid state NMR spectroscopy and accurate first-principles calculations. *Geochimica Et Cosmochimica Acta* , **2014**, 125, 170-185	5.5	55
106	Study of the structural role of gallium and aluminum in 45S5 bioactive glasses by molecular dynamics simulations. *Journal of Physical Chemistry B*, **2013**, 117, 4142-50	3.4	55
105	Unambiguous Description of the Oxygen Environment in Multicomponent Aluminosilicate Glasses from 17O Solid State NMR Computational Spectroscopy. *Journal of Physical Chemistry C*, **2012**, 116, 14599-14609	3.8	51
104	Fluorescence spectra of organic dyes in solution: a time dependent multilevel approach. *Physical Chemistry Chemical Physics*, **2011**, 13, 2160-6	3.6	51
103	Medium-range order in phospho-silicate bioactive glasses: Insights from MAS-NMR spectra, chemical durability experiments and molecular dynamics simulations. *Journal of Non-Crystalline Solids*, **2008**, 354, 84-89	3.9	50
102	Environmental effects in computational spectroscopy: accuracy and interpretation. *ChemPhysChem*, **2010**, 11, 1812-32	3.2	47
101	Properties of zinc releasing surfaces for clinical applications. *Journal of Biomaterials Applications*, **2008**, 22, 505-26	2.9	46
100	Assessment of Exchange-Correlation Functionals in Reproducing the Structure and Optical Gap of Organic-Protected Gold Nanoclusters. *Journal of Physical Chemistry C*, **2014**, 118, 7532-7544	3.8	45
99	Role of Host□Guest Interactions in Tuning the Optical Properties of Coumarin Derivatives Incorporated in MCM-41: A TD-DFT Investigation. *Journal of Physical Chemistry C*, **2012**, 116, 17807-17818	3.8	43
98	B3LYP Simulation of the Full Vibrational Spectrum of 45S5 Bioactive Silicate Glass Compared to v-Silica. *Chemistry of Materials*, **2008**, 20, 5610-5621	9.6	42
97	Large-Scale B3LYP Simulations of Ibuprofen Adsorbed in MCM-41 Mesoporous Silica as Drug Delivery System. *Journal of Physical Chemistry C*, **2014**, 118, 26737-26749	3.8	41
96	Theoretical multilevel approach for studying the photophysical properties of organic dyes in solution. *Physical Chemistry Chemical Physics*, **2010**, 12, 10550-61	3.6	41

95	A closer look into the ubiquitin corona on gold nanoparticles by computational studies. *New Journal of Chemistry*, **2015**, 39, 2474-2482	3.6	40
94	Elastic and dynamical properties of alkali-silicate glasses from computer simulations techniques. *Theoretical Chemistry Accounts*, **2008**, 120, 557-564	1.9	40
93	Computational Protocol for Modeling Thermochromic Molecular Crystals: Salicylidene Aniline As a Case Study. *Journal of Chemical Theory and Computation*, **2014**, 10, 5577-85	6.4	39
92	Unraveling solvent effects on the electronic absorption spectra of TRITC fluorophore in solution: a theoretical TD-DFT/PCM study. *Physical Chemistry Chemical Physics*, **2010**, 12, 2722-9	3.6	38
91	Understanding Aggregation-Induced Emission in Molecular Crystals: Insights from Theory. *Journal of Physical Chemistry C*, **2017**, 121, 5747-5752	3.8	37
90	Absorption and emission spectra of fluorescent silica nanoparticles from TD-DFT/MM/PCM calculations. *Physical Chemistry Chemical Physics*, **2011**, 13, 16689-97	3.6	34
89	Insight into the structure of vanadium containing glasses: A molecular dynamics study. *Journal of Non-Crystalline Solids*, **2011**, 357, 2571-2579	3.9	34
88	The effect of composition on structural, thermal, redox and bioactive properties of Ce-containing glasses. *Materials and Design*, **2016**, 97, 73-85	8.1	33
87	Interplay of stereo-electronic, environmental, and dynamical effects in determining the EPR parameters of aromatic spin-probes: INDCO as a test case. *Physical Chemistry Chemical Physics*, **2010**, 12, 3741-6	3.6	33
86	An integrated computational protocol for the accurate prediction of EPR and PNMR parameters of aminoxyl radicals in solution. *Magnetic Resonance in Chemistry*, **2010**, 48 Suppl 1, S11-22	2.1	33
85	Influence of Silver Doping on the Photoluminescence of Protected AgnAu25□ Nanoclusters: A Time-Dependent Density Functional Theory Investigation. *Journal of Physical Chemistry C*, **2015**, 119, 10766-10775	3.8	32
84	Calcium environment in silicate and aluminosilicate glasses probed by □Ca MQMAS NMR experiments and MD-GIPAW calculations. *Solid State Nuclear Magnetic Resonance*, **2015**, 68-69, 31-6	3.1	31
83	First-principles simulations of the 27Al and 17O solid-state NMR spectra of the CaAl2Si3O10 glass. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	31
82	An ab initio parameterized interatomic force field for hydroxyapatite. *Journal of Materials Chemistry*, **2007**, 17, 2061		31
81	Two-Dimensional Electronic Spectroscopy Reveals Dynamics and Mechanisms of Solvent-Driven Inertial Relaxation in Polar BODIPY Dyes. *Journal of Physical Chemistry Letters*, **2018**, 9, 1079-1085	6.4	30
80	Understanding the photophysical properties of coumarin-based Pluronic-silica (PluS) nanoparticles by means of time-resolved emission spectroscopy and accurate TDDFT/stochastic calculations. *Physical Chemistry Chemical Physics*, **2013**, 15, 12360-72	3.6	29
79	A computational multiscale strategy to the study of amorphous materials. *Theoretical Chemistry Accounts*, **2007**, 117, 933-942	1.9	29
78	A computational tool for the prediction of crystalline phases obtained from controlled crystallization of glasses. *Journal of Physical Chemistry B*, **2005**, 109, 21586-92	3.4	29

77	Effects of Substituents on Transport Properties of Molecular Materials for Organic Solar Cells: A Theoretical Investigation. *Chemistry of Materials*, **2017**, 29, 673-681	9.6	28
76	DFT and TD-DFT assessment of the structural and optoelectronic properties of an organic-Ag14 nanocluster. *Journal of Physical Chemistry A*, **2015**, 119, 5088-98	2.8	27
75	Computational interpretation of 23Na MQMAS NMR spectra: A comprehensive investigation of the Na environment in silicate glasses. *Chemical Physics Letters*, **2014**, 612, 56-61	2.5	27
74	Accurate First-Principle Prediction of (29)Si and (17)O NMR Parameters in SiO2 Polymorphs: The Cases of Zeolites Sigma-2 and Ferrierite. *Journal of Chemical Theory and Computation*, **2008**, 4, 2130-40	6.4	26
73	Raman and DFT study of methimazole chemisorbed on gold colloidal nanoparticles. *Physical Chemistry Chemical Physics*, **2016**, 18, 5974-80	3.6	23
72	Molecular dynamics simulations of sodium silicate glasses: Optimization and limits of the computational procedure. *Computational Materials Science*, **2010**, 47, 739-751	3.2	23
71	Insights into structural and dynamical features of water at halloysite interfaces probed by DFT and classical molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2016**, 18, 2164-74	3.6	22
70	Oxalyl dihydrazide polymorphism: a periodic dispersion-corrected DFT and MP2 investigation. *CrystEngComm*, **2014**, 16, 102-109	3.3	22
69	Vibrational features of phospho-silicate glasses: Periodic B3LYP simulations. *Chemical Physics Letters*, **2009**, 476, 218-222	2.5	22
68	Magneto-Plasmonic Colloidal Nanoparticles Obtained by Laser Ablation of Nickel and Silver Targets in Water. *Journal of Physical Chemistry C*, **2017**, 121, 3597-3606	3.8	21
67	Computational Insight into the Effect of Natural Compounds on the Destabilization of Preformed Amyloid-[1?40) Fibrils. *Molecules*, **2018**, 23,	4.8	21
66	Multiscale Molecular Dynamics Simulation of Multiple Protein Adsorption on Gold Nanoparticles. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	21
65	Modeling emission features of salicylidene aniline molecular crystals: A QM/QM' approach. *Journal of Computational Chemistry*, **2016**, 37, 861-70	3.5	21
64	Experimental and DFT Characterization of Halloysite Nanotubes Loaded with Salicylic Acid. *Journal of Physical Chemistry C*, **2016**, 120, 26759-26769	3.8	21
63	Environmental and dynamical effects on the optical properties of molecular systems by time-independent and time-dependent approaches: Coumarin derivatives as test cases. *Computational and Theoretical Chemistry*, **2014**, 1037, 35-48	2	20
62	Molecular Dynamics Investigation of Halide-Containing Phospho-Silicate Bioactive Glasses. *Journal of Physical Chemistry B*, **2018**, 122, 2940-2948	3.4	19
61	SERS, XPS and DFT Study of Xanthine Adsorbed on Citrate-Stabilized Gold Nanoparticles. *Sensors*, **2019**, 19,	3.8	19
60	DFT modeling of 45S5 and 77S soda-lime phospho-silicate glass surfaces: clues on different bioactivity mechanism. *Langmuir*, **2013**, 29, 5749-59	4	19

59	Towards a quantitative rationalization of multicomponent glass properties by means of molecular dynamics simulations. *Molecular Simulation*, **2006**, 32, 1045-1055	2	19
58	Recent advances in solid-state NMR computational spectroscopy: The case of alumino-silicate glasses. *International Journal of Quantum Chemistry*, **2016**, 116, 1520-1531	2.1	19
57	Dynamics of Fracture in Silica and Soda-Silicate Glasses: From Bulk Materials to Nanowires. *Journal of Physical Chemistry C*, **2015**, 119, 25499-25507	3.8	18
56	Structural origins of the Mixed Alkali Effect in Alkali Aluminosilicate Glasses: Molecular Dynamics Study and its Assessment. *Scientific Reports*, **2020**, 10, 2906	4.9	18
55	Assessment of interatomic parameters for the reproduction of borosilicate glass structures via DFT-GIPAW calculations. *Journal of the American Ceramic Society*, **2019**, 102, 7225-7243	3.8	18
54	On the structure of Ce-containing silicophosphate glasses: a core-shell molecular dynamics investigation. *Physical Chemistry Chemical Physics*, **2014**, 16, 21645-56	3.6	18
53	On the opto-electronic properties of phosphine and thiolate-protected undecagold nanoclusters. *Physical Chemistry Chemical Physics*, **2014**, 16, 18749-58	3.6	18
52	The electronic structure of the lutein triplet state in plant light-harvesting complex II. *Physical Chemistry Chemical Physics*, **2012**, 14, 12238-51	3.6	18
51	Deflocculant effects on the surface properties of kaolinite investigated through malachite green adsorption. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2008**, 329, 31-37	5.1	18
50	A Modular Implementation for the Simulation of 1D and 2D Solid-State NMR Spectra of Quadrupolar Nuclei in the Virtual Multifrequency Spectrometer-Draw Graphical Interface. *Journal of Chemical Theory and Computation*, **2017**, 13, 2215-2229	6.4	17
49	Assessment of Density Functional Approximations for Highly Correlated Oxides: The Case of CeO and CeO. *Journal of Chemical Theory and Computation*, **2018**, 14, 4914-4927	6.4	17
48	On the simulation of vibrationally resolved electronic spectra of medium-size molecules: the case of styryl substituted BODIPYs. *Physical Chemistry Chemical Physics*, **2019**, 21, 3512-3526	3.6	17
47	On the ability of periodic dispersion-corrected DFT calculations to predict molecular crystal polymorphism in para-diiodobenzene. *Chemical Physics Letters*, **2012**, 541, 12-15	2.5	17
46	Crystallization kinetics of bioactive glasses in the ZnO-Na2O-CaO-SiO2 system. *Journal of Physical Chemistry A*, **2007**, 111, 8401-8	2.8	17
45	Computational Insight into the Interaction of Cytochrome C with Wet and PVP-Coated Ag Surfaces. *Journal of Physical Chemistry B*, **2017**, 121, 9532-9540	3.4	15
44	New insights into the bioactivity of SiO2□CaO and SiO2□CaO□P2O5 sol□gel glasses by molecular dynamics simulations. *Journal of Sol-Gel Science and Technology*, **2013**, 67, 208-219	2.3	15
43	Local versus Average Structure in LaSrAl3O7: A NMR and DFT Investigation. *Journal of Physical Chemistry C*, **2013**, 117, 23451-23458	3.8	15
42	Extension of the AMBER force field to cyclic □,□-dialkylated peptides. *Physical Chemistry Chemical Physics*, **2012**, 14, 15308-20	3.6	14

41	Optical properties of the dibenzothiazolylphenol molecular crystals through ONIOM calculations: the effect of the electrostatic embedding scheme. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	13
40	Models of Aged Magnesium Silicate Hydrate Cements Based on the Lizardite and Talc Crystals: A Periodic DFT-GIPAW Investigation. *Journal of Physical Chemistry C*, **2017**, 121, 7319-7330	3.8	12
39	Role of specific solute-solvent interactions on the photophysical properties of distyryl substituted BODIPY derivatives. *Physical Chemistry Chemical Physics*, **2020**, 22, 10981-10994	3.6	12
38	Supercritical CO2Confined in Palygorskite and Sepiolite Minerals: A Classical Molecular Dynamics Investigation. *Journal of Physical Chemistry C*, **2016**, 120, 26945-26954	3.8	12
37	Structure of active cerium sites within bioactive glasses. *Journal of the American Ceramic Society*, **2017**, 100, 5086-5095	3.8	12
36	Density of multicomponent silica-based potential bioglasses: Quantitative structure-property relationships (QSPR) analysis. *Journal of the European Ceramic Society*, **2007**, 27, 499-504	6	12
35	Insights into the Effect of Curcumin and (-)-Epigallocatechin-3-Gallate on the Aggregation of A(1-40) Monomers by Means of Molecular Dynamics. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	12
34	Structure Model and Toxicity of the Product of Biodissolution of Chrysotile Asbestos in the Lungs. *Chemical Research in Toxicology*, **2019**, 32, 2063-2077	4	11
33	Computational Modeling of Silicate Glasses: A Quantitative Structure-Property Relationship Perspective. *Springer Series in Materials Science*, **2015**, 113-135	0.9	11
32	Unraveling the polymorphism of [(p-cymene)Ru(N-INA)Cl]through dispersion-corrected DFT and NMR GIPAW calculations. *Inorganic Chemistry*, **2014**, 53, 7926-35	5.1	11
31	Electronic and optical properties of the Au22[1,8-bis(diphenylphosphino) octane]6 nanoclusters disclosed by DFT and TD-DFT calculations. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	10
30	Computational Insights into the Binding of Monolayer-Capped Gold Nanoparticles onto Amyloid- Fibrils. *ACS Chemical Neuroscience*, **2020**, 11, 3153-3160	5.7	9
29	Raman and Computational Study on the Adsorption of Xanthine on Silver Nanocolloids. *ACS Omega*, **2018**, 3, 13530-13537	3.9	9
28	New Insight into Mixing Fluoride and Chloride in Bioactive Silicate Glasses. *Scientific Reports*, **2018**, 8, 1316	4.9	8
27	Combined Experimental and Computational Approach toward the Structural Design of Borosilicate-Based Bioactive Glasses. *Journal of Physical Chemistry C*, **2020**, 124, 17655-17674	3.8	8
26	Disclosing crystal nucleation mechanism in lithium disilicate glass through molecular dynamics simulations and free-energy calculations. *Scientific Reports*, **2020**, 10, 17867	4.9	7
25	SERS active Ag-SiO nanoparticles obtained by laser ablation of silver in colloidal silica. *Beilstein Journal of Nanotechnology*, **2018**, 9, 2396-2404	3	7
24	H2 Dissociation and Water Evolution on Silver-Decorated CeO2(111): A Hybrid Density Functional Theory Investigation. *Journal of Physical Chemistry C*, **2019**, 123, 25668-25679	3.8	6

23	O2 Activation over Ag-Decorated CeO2(111) and TiO2(110) Surfaces: A Theoretical Comparative Investigation. *Journal of Physical Chemistry C*, **2020**, 124, 25917-25930	3.8	6
22	An atomic-level look at the structure-property relationship of cerium-doped glasses using classical molecular dynamics. *Journal of Non-Crystalline Solids*, **2018**, 498, 331-337	3.9	4
21	Adsorption of Trans-Zeatin on Laser-Ablated Gold Nanoparticles for Transport into Plant Cells and Growth Stimulation. *ACS Applied Nano Materials*, **2019**, 2, 7319-7327	5.6	4
20	Experimental and Molecular Dynamics Investigation Proves That Montmorillonite Traps the Biogenic Amines Histamine and Tyramine. *Journal of Physical Chemistry C*, **2017**, 121, 27493-27503	3.8	4
19	Disclosing the Interaction of Gold Nanoparticles with A[1-40) Monomers through Replica Exchange Molecular Dynamics Simulations. *International Journal of Molecular Sciences*, **2020**, 22,	6.3	4
18	Exploring the crystallization path of lithium disilicate through metadynamics simulations. *Physical Review Materials*, **2021**, 5,	3.2	4
17	Assessment of the basis set effect on the structural and electronic properties of organic-protected gold nanoclusters. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	4
16	Reducibility of Ag- and Cu-Modified Ultrathin Epitaxial Cerium Oxide Films. *Journal of Physical Chemistry C*, **2019**, 123, 13702-13711	3.8	3
15	In Silico Study of Hydroxyapatite and Bioglass : How Computational Science Sheds Light on Biomaterials **2011**,		3
14	Toward the understanding of crystallization, mechanical properties and reactivity of multicomponent bioactive glasses. *Acta Materialia*, **2021**, 213, 116977	8.4	3
13	The antioxidant properties of Ce-containing bioactive glass nanoparticles explained by Molecular Dynamics simulations. *Biomedical Glasses*, **2016**, 2,	2.7	2
12	The Effect of Alkaline Cations on the Intercalation of Carbon Dioxide in Sepiolite Minerals: A Molecular Dynamics Investigation. *Frontiers in Materials*, **2018**, 5,	4	2
11	Development and Application of a ReaxFF Reactive Force Field for Cerium Oxide/Water Interfaces. *Journal of Physical Chemistry A*, **2021**, 125, 5693-5708	2.8	2
10	Spectroscopic and Computational Studies on Ligand-Capped Metal Nanoparticles and Clusters **2018**, 55-87		2
9	Reprint of Environmental and dynamical effects on the optical properties of molecular systems by time-independent and time-dependent approaches: Coumarin derivatives as test cases *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 144-157	2	1
8	Magnetic Resonance Spectroscopy: Singlet and Doublet Electronic States **2011**, 207-248		1
7	Unraveling the internal conversion process within the Q-bands of a chlorophyll-like-system through surface-hopping molecular dynamics simulations. *Journal of Chemical Physics*, **2021**, 154, 094110	3.9	1
6	Improved empirical force field for multicomponent oxide glasses and crystals. *Physical Review Materials*, **2021**, 5,	3.2	1

List of Publications

5	What Can We Learn from Atomistic Simulations of Bioactive Glasses?. *Advanced Structured Materials*, **2016**, 119-145	0.6	1
4	Structure Analysis and Properties Calculations **2022**, 89-122		0
3	The effect of the incorporation of catalase mimetic activity cations on the structural, thermal and chemical durability properties of the 45S5 Bioglass . *Acta Materialia*, **2022**, 229, 117801	8.4	0
2	First-principles simulations of the 27Al and 17O solid-state NMR spectra of the CaAl2Si3O10 glass. *Highlights in Theoretical Chemistry*, **2013**, 87-97		
1	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. *Highlights in Theoretical Chemistry*, **2013**, 319-337		